

University of Groningen

Low exciton binding energies from computational predictions

de Gier, Hilde Dorothea

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version

Publisher's PDF, also known as Version of record

Publication date:

2016

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

de Gier, H. D. (2016). *Low exciton binding energies from computational predictions: Towards the next generation of organic photovoltaics*. [Thesis fully internal (DIV), University of Groningen]. University of Groningen.

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

ACK

Acknowledgements

This thesis marks for me the end of a period of education at the University of Groningen. Many people have contributed to these years. I would like to mention here those who were involved during my four years as a PhD candidate.

First of all, I would like to thank my daily supervisor and copromotor Remco Havenith for his commitment to my PhD project. I acknowledge your clear explanation of the theory and your programming and user experience with a wide variety of software packages for electronic structure calculations. Thank you for your bright ideas that improved the content of my presentations, publications and this thesis. I hope my project may be a starting point for your ‘next generation’ of students in the field of organic photovoltaics.

My thanks also go to my first promotor Ria Broer for her valuable ideas and contributions to my PhD. Your criticism really improved the quality of my scientific work. I acknowledge your great comprehension of the *ab initio* methods. It is to be wished that the research conducted in your group will profit by my project. Thank you for having accepted me as a member of the Theoretical Chemistry group.

I am grateful to my second promotor Kees Hummelen for his scientific contribution to my PhD research and his useful suggestions. I learned a lot from your great knowledge about organic photovoltaics. Your enthusiasm for organic solar cells certainly got me energised for this topic! I hope my results will prove to be valuable for the future research within the FOM-focus group. Thank you for having accepted me as a member.

I would like to express my gratitude to the members of the Assessment Committee, Prof. Siewert-Jan Marrink, Prof. Andries Meijerink and Prof. Mark A. Ratner, for having carefully read my thesis and for their interest in my research.

I thank all current and previous members of the Theoretical Chemistry group for their share in a pleasant work environment. Special thanks go to my PhD colleague Gerrit-Jan Linker for his sympathy for me and my research, and for the nice time we spent together at conferences and schools. I keep ‘more or less’ warm memories of our participation in the European summer school in Quantum Chemistry on Sicily in September 2013 and in the winter school in Theoretical Chemistry and Spectroscopy in Han-sur-Lesse in December 2012 and 2014! I cordially thank Wim Nieuwpoort and Piet van Duijnen for many useful discussions during the group meetings and otherwise.

I would also like to thank the two dedicated master students whom I supervised during my PhD, Bernd Rietberg and Neus Aguilera, for the interesting discussions and for their contributions to several parts of my research.

All current and previous members of the FOM-focus group: thank you for your input in the bi-weekly scientific meetings. My special thanks go to Jan-Anton Koster for his interest in my PhD research and for many useful discussions. I thank Mehrnoosh Jahani for her contribution to Chapter 4 of this thesis.

The research in this thesis greatly benefitted from the discussions I had with several scientists working at the Zernike Institute for Advanced Materials, in particular Alex de Vries and Maxim Pchenitchnikov. My special thanks go to the director of the Graduate School of Science, Petra Rudolf.

I would like to thank the secretaries Henriët van Mil-Boddevelde and Renate Hekkema-Nieborg for their friendly support during the four years of my PhD.

I thank the staff of the Donald Smits Center for Information Technology at the University of Groningen, in particular Fokke Dijkstra and Ger Strikwerda, the staff of SURFsara in Amsterdam and the staff of Oak Ridge Leadership Computing Facility (OLCF) in the USA for assisting with computations on the Millipede cluster at the University of Groningen, the Dutch National Supercomputers Huygens and Cartesius at SURFsara, and the Titan Supercomputer at OLCF.

My thanks also go to my employer Stichting FOM for investing in my professional development through courses for PhD students and conferences. I learned a lot from the coaches and the interaction with my fellow FOM PhD students during these meetings. Although I had to travel more than two hours, this time investment was always worthwhile!

I would like to thank Gerrit-Jan Linker and Gonda de Gier for helping me with the preparations for the PhD defence. I am honoured that you have accepted to be my paranymphs.

Last, but not least, I would like to express my deep gratitude to my family for their unconditional caring, moral support and understanding. Thank you for being there for me every step of the way.

Hilde D. de Gier

